Cyclohexane 110-82-7 | DTXSID4021923

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 59.1

Global applicability domain: Inside

Local applicability domain index: 5.20e-01

Confidence level: 6.57e-01

Nearest Neighbors from the Training Set

Image not found

Cyclohexane Measured: 83.2 Predicted: 59.1 Image not found

Methylcyclohexane Measured: 186 Predicted: 233 Image not found

Butyl ether Measured: 72.4 Predicted: 32.3

Image not found

Quinoline Measured: 3.80 Predicted: 6.66 Image not found

Benzene Measured: 4.27 Predicted: 10.0